ABSTRACT

A three-dimensional quantitative structure-activity relationship method has process B1 of calculating the coordinates of the respective atoms contained in the plural molecules thus superposed in the virtual space, process B2 of calculating interatomic distances between each atom and other atoms and identifying the shortest interatomic distance among thus calculated interatomic distances and two atoms constituting the shortest interatomic distance; process B3 of deleting the two atoms having the shortest interatomic distance from the three-dimensional space and generating an atom which represents the two atoms in the weighted average coordinates of the two atoms to delete, when the shortest interatomic distance thus calculated is equal to or smaller than a predetermined threshold value; process B4 of returning to the second process B2 after the third process B3 and executing the second process B2 including the atoms formed during the third process B3; and process B5 of terminating the process B when the shortest interatomic distance thus calculated is exceeds the predetermined threshold. This method enables strikingly reducing the memory zone and amount of computation required for 3D QSAR analysis.